Growth of Iron on GaAs

Theory and Practice

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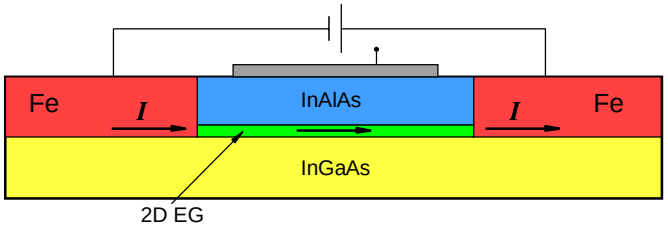
Spintronics and Fe/GaAs

Magnetic nanostructure technologies

- Non-volatile magnetic storage devices
  - Patterned magnetic media: "quantized magnetic disks"
  - Magnetic random-access memories (MRAM)
- Spin-injection devices
  - Spin valves
  - Spin RTDs & filters
  - Spin FETs



Spin-polarized FET
Datta & Das, APL 1990

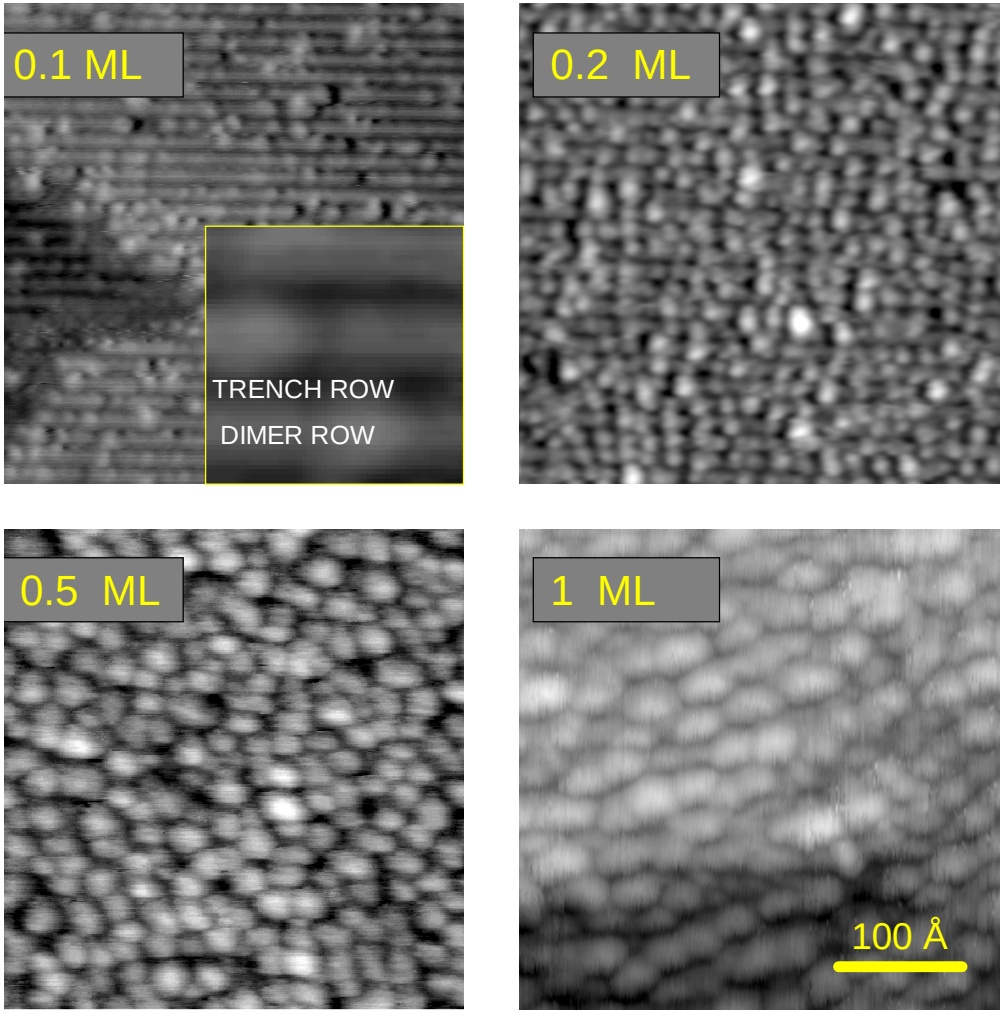
Fe/GaAs: Questions for surface science

- Structural properties
  - How does Fe grow on GaAs(001) in the submonlayer regime?
  - What role does surface diffusion play in the initial stages of growth?
  - How does the Fe/GaAs interface depend on the surface reconstruction?
  - Does Fe grow layer-by-layer or by forming islands?
- Magnetic properties
  - What interplay is there betwen magnetism and chemistry?
  - How does magnetism develop in the first few layers?

This talk

Initial stages of growth: STM images

Fe deposited on As-rich GaAs(001)-(2x4) at 175 °C



*.M. Thibado et al., Phys. Rev. B **53**, R10481 (1995)*

GaAs(001)-(2x4) substrate

- Surface terminated by As dimers
- STM: Bright double-dimer rows separated by dark trenches

Low coverage Fe deposition

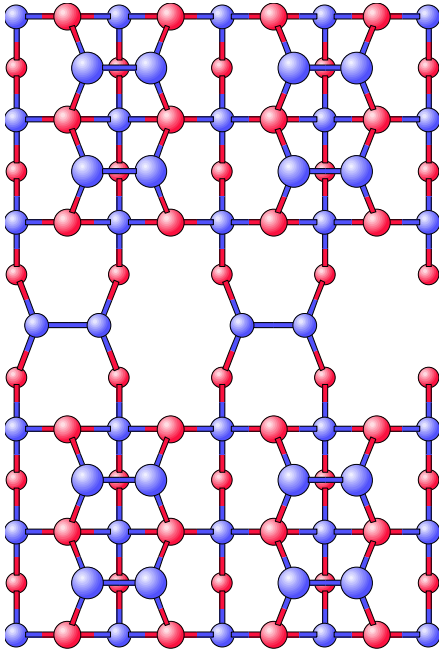
- 0.1 ML: Small 2D Fe islands nucleate on As-dimer rows
- 0.2 ML: Fe islands still confined to As dimer rows
- 0.5 ML: Elongation of islands along dimer rows; trenches begin to fill in
- 1 ML: Elongation continues along dimer rows; second Fe layer begins to grow

The substrate: As-rich GaAs(001)

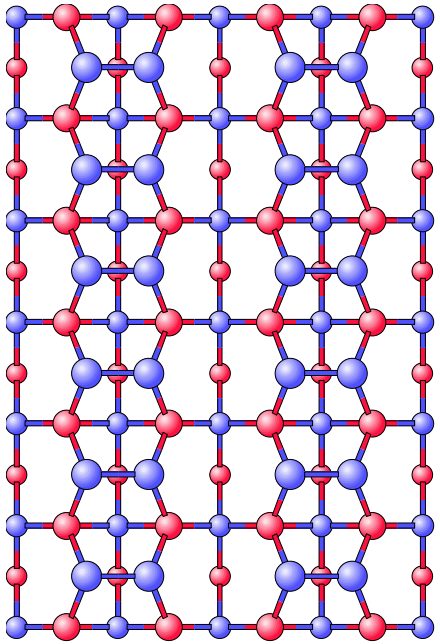
Actual ß2(2x4) reconstruction

Fictitious (2x1) reconstruction

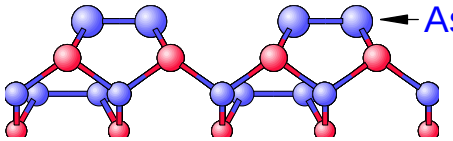
Top view

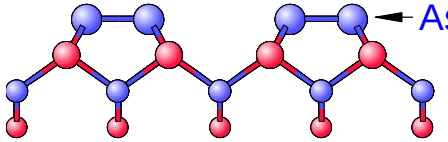


computational simplification



ide view





Surface terminated by As dimers
As double-dimer rows separated by trenches
Trenches also terminated by As dimers

Surface terminated by As dimers
No trenches

Local geometry & chemistry unchanged

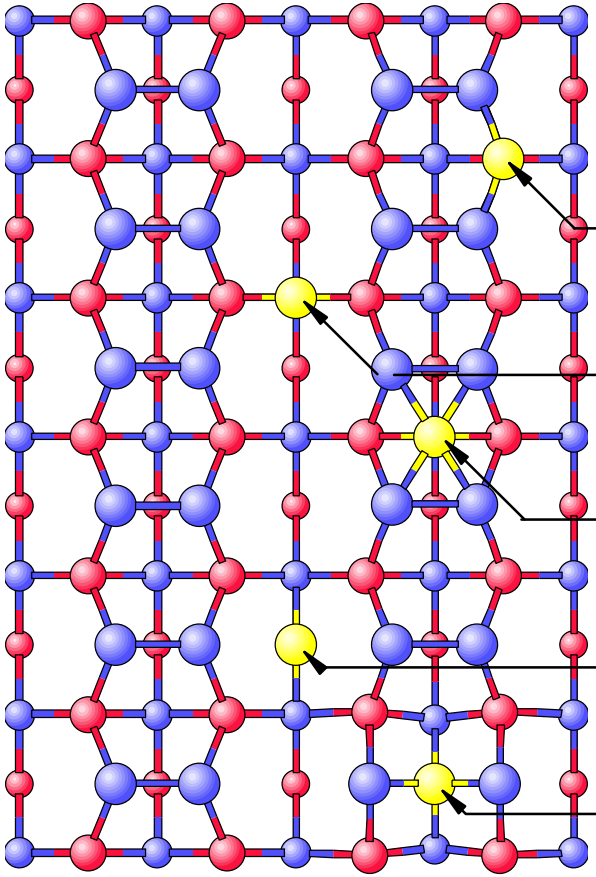
Computational details

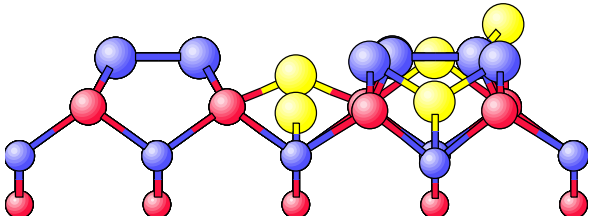
Supercell geometry	6 layers GaAs, terminated by pseudo-H
Structural relaxation	topmost 3-5 layers

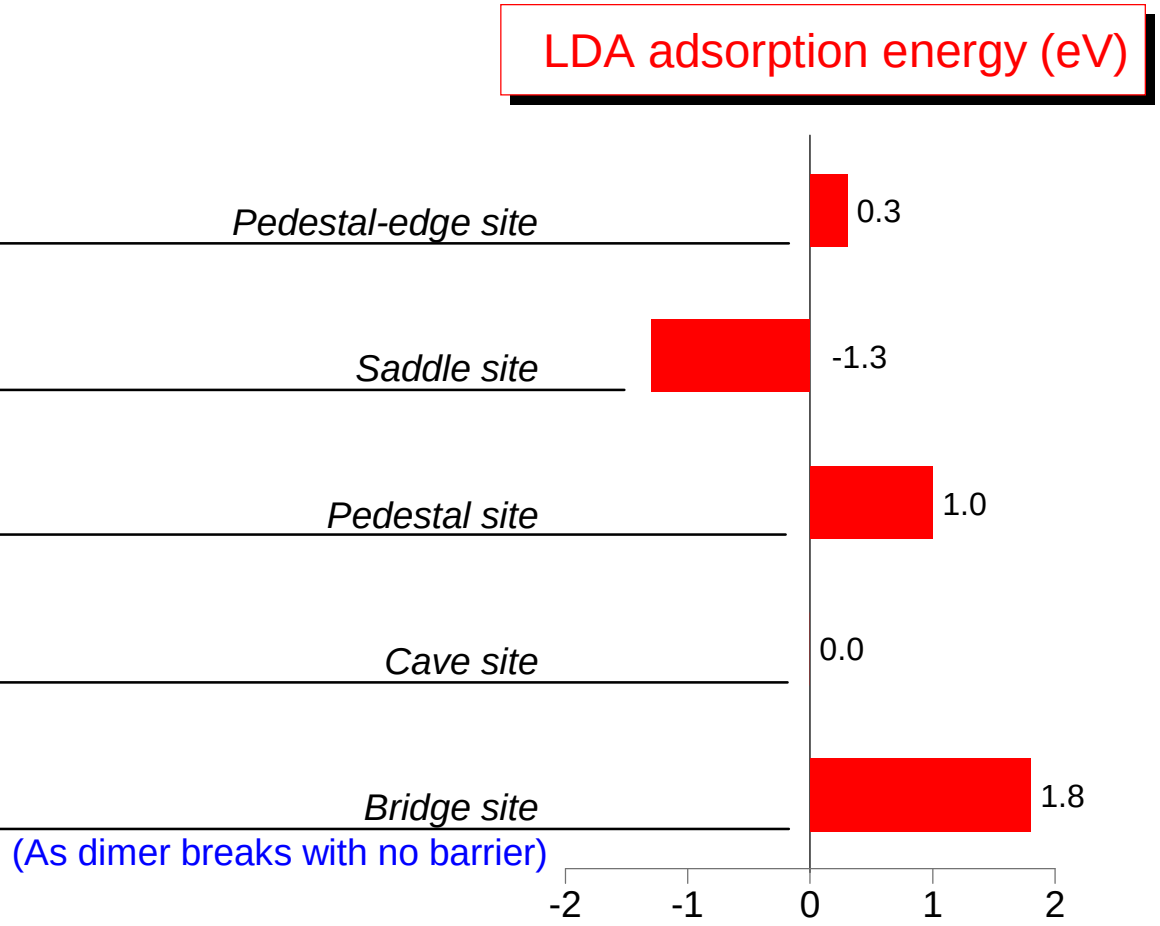
Theoretical method	Local-(Spin-)Density Approximation + GGA
Electron-ion interaction	Troullier-Martins pseudopotentials
lane-wave energy cutoff	50 Rydbergs
Brillouin-zone sampling	equivalent to 64 k-points/1x1-cell

Computer software	FHI96MD (Bockstedte, Kley, Neugebauer & Scheffler)

Fe adsorption: Isolated atoms



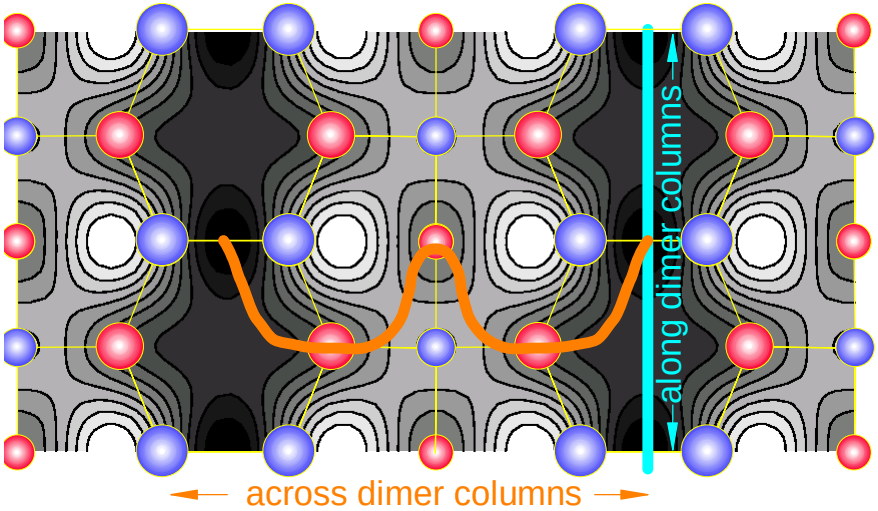


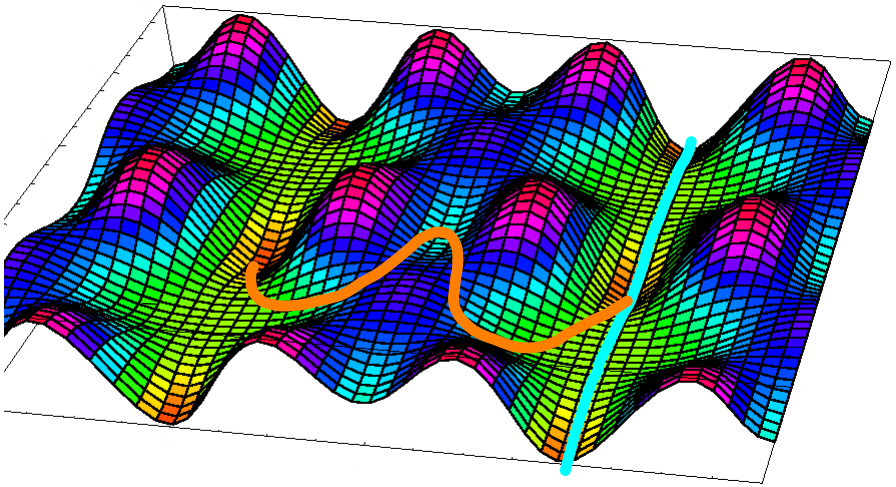


Bridge site: the key to growth?

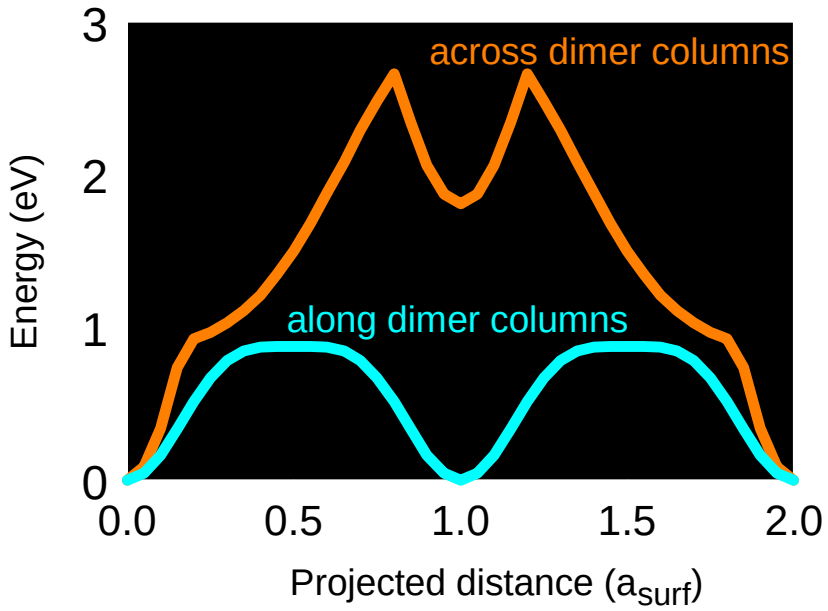
- Most favorable binding site by ~1 eV
- Barrierless unreconstruction of substrate

Potential energy surface for Fe adatoms





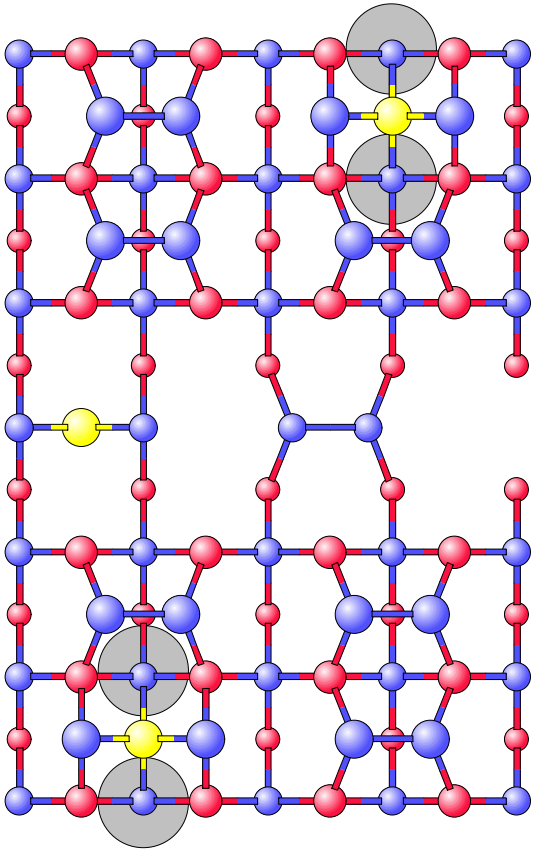
Lowest-energy diffusion pathways

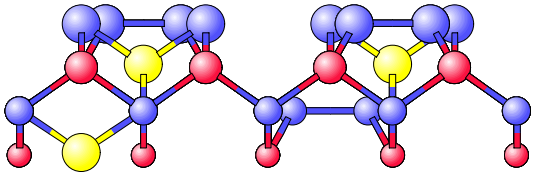


Highly anisotropic diffusion barriers

- Across As dimer columns: ~3 eV
- Along As dimer columns: ~1 eV

Ideal growth: A simple scenario





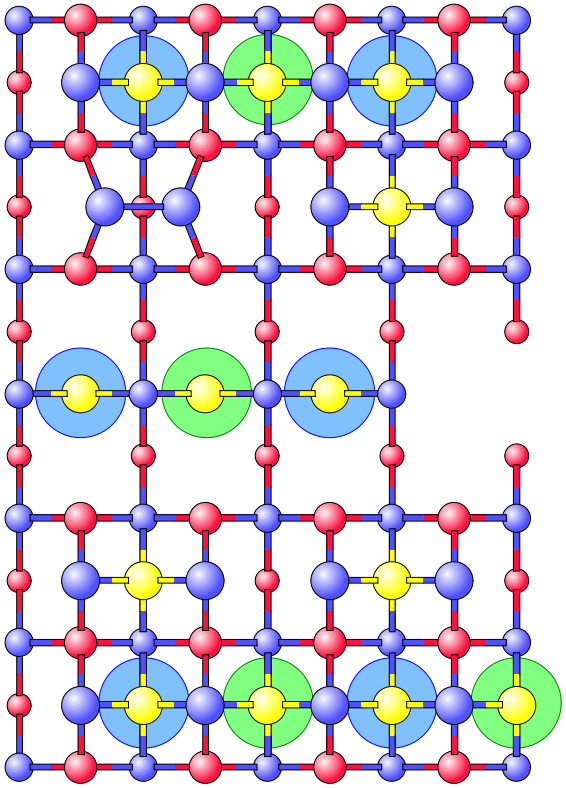
Diffusion

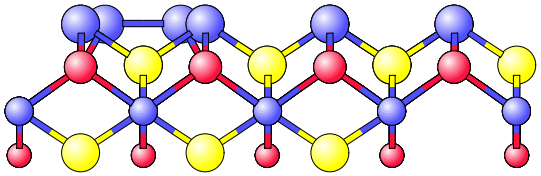
- Fe adatoms diffuse along As-dimer columns

Adsorption

- Fe adatoms bind to As-bridge sites
- Ideal substrate locally restored
- Adsorption blocked at pedestal sites:

Ideal growth (Phase 2)

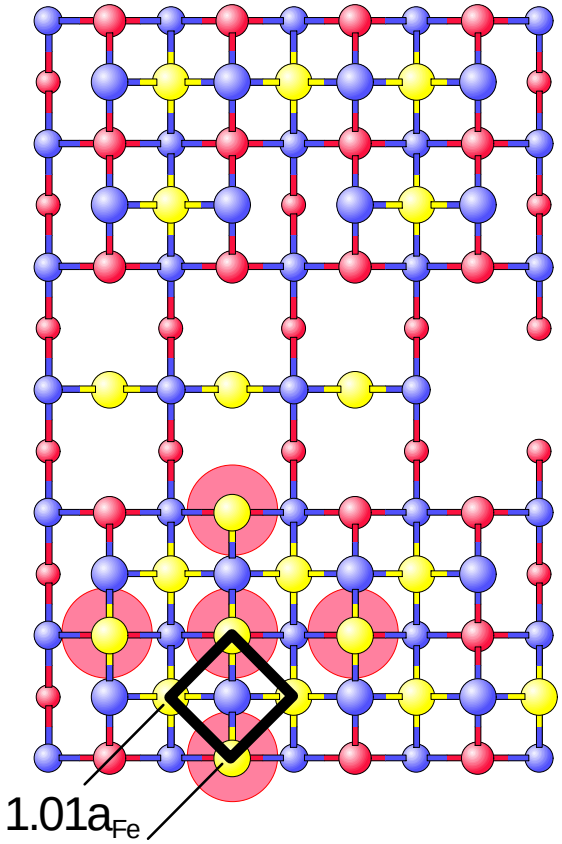


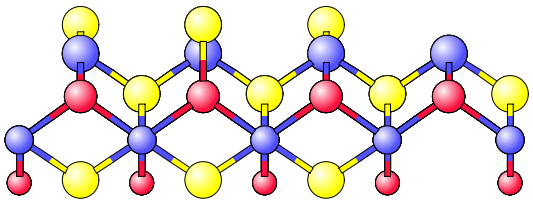


"Promoted" adsorption

- Fe on 2 adjacent bridge sites...
- ...converts a cave site to a bridge site

Ideal growth (Phase 3)



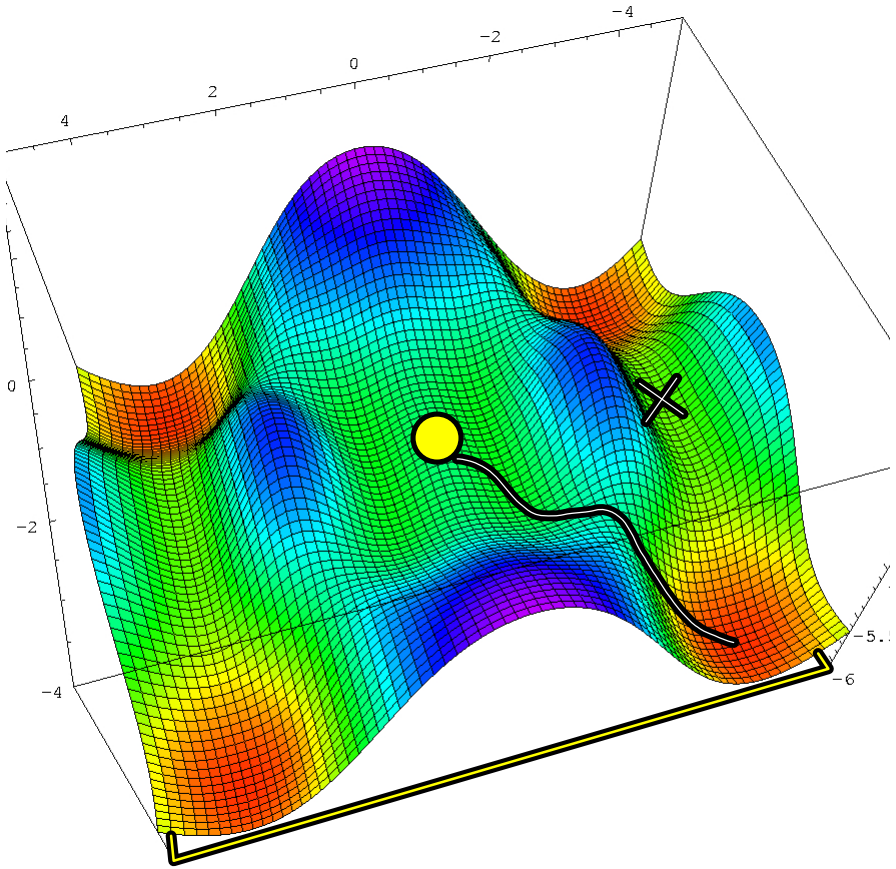


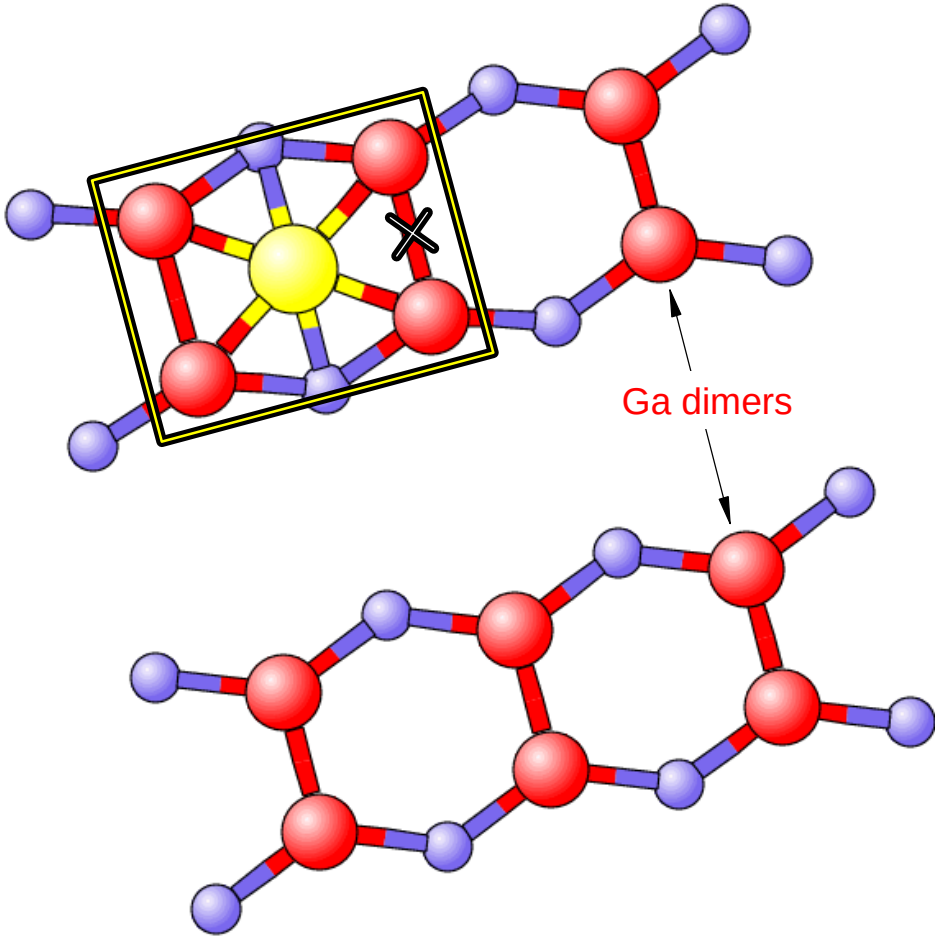
Coverage between 1 and 2 MLs

- Fe adatoms begin to occupy pedestal-edge sites
- ⇒ Highly corrugated bcc-Fe basal plane?

Growth on Ga-rich GaAs(001)

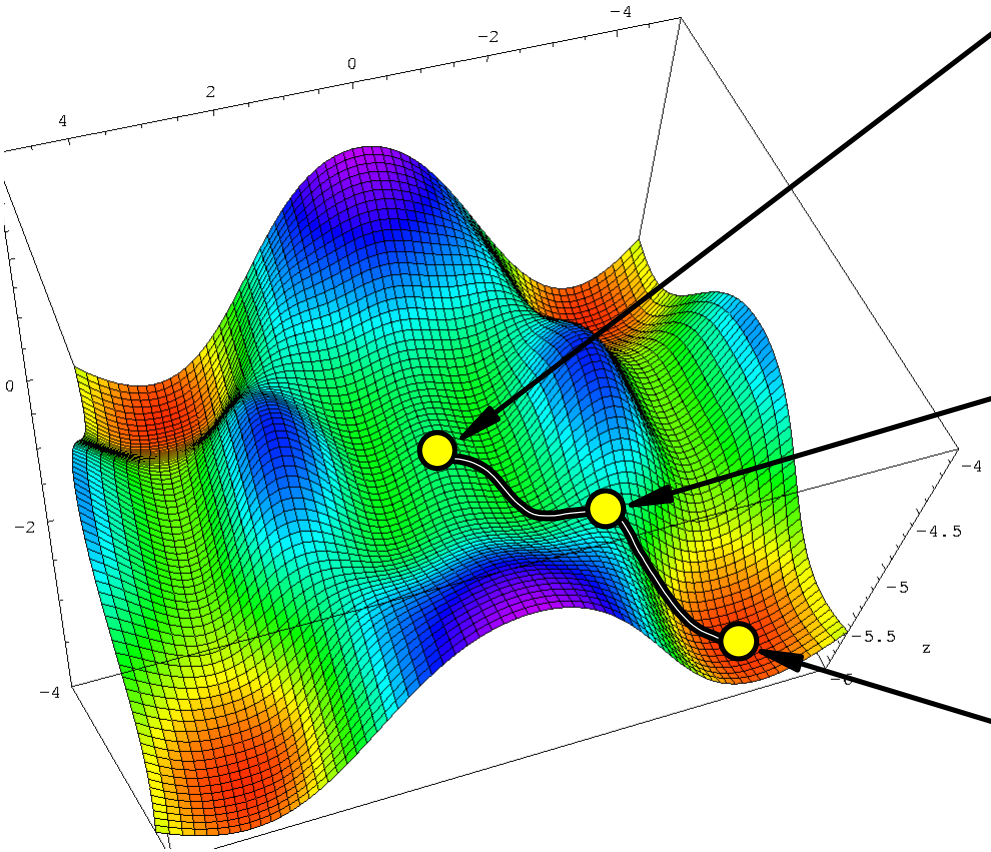
Potential energy surface near pedestal site



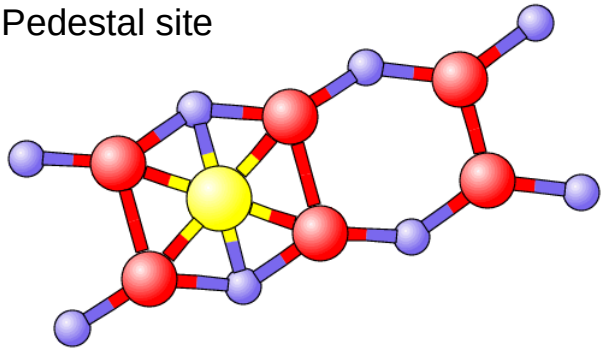


Critical points on the reaction path

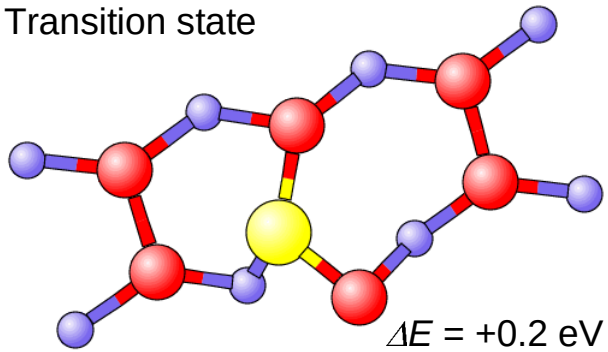
First stage of Fe film growth



Pedestal site

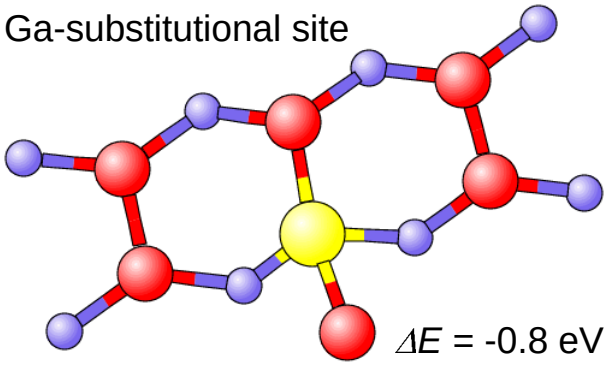


Transition state



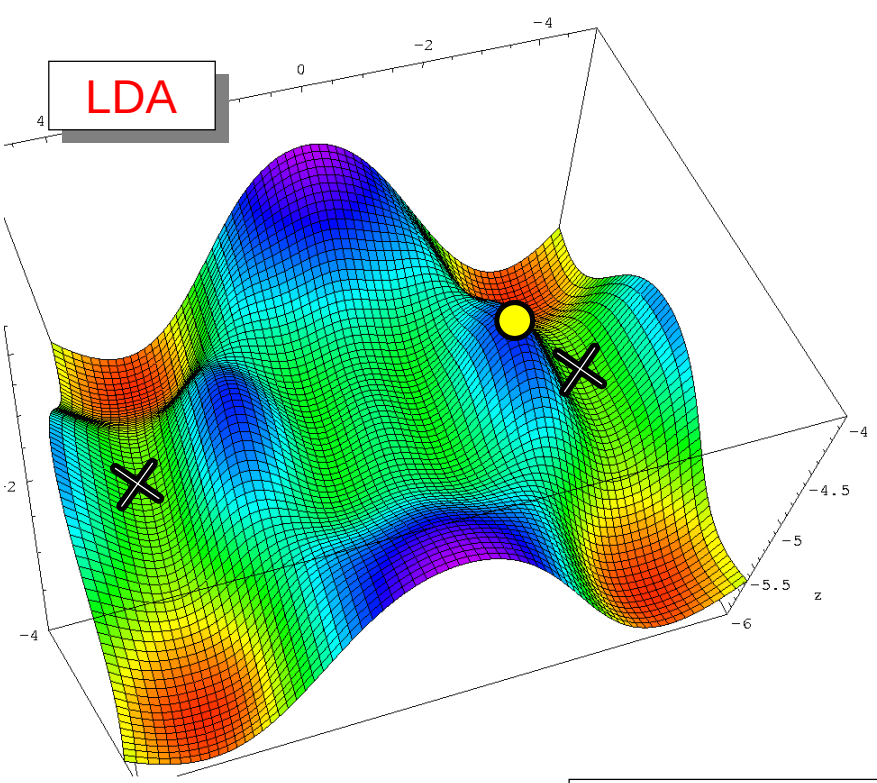
ΔE = +0.2 eV

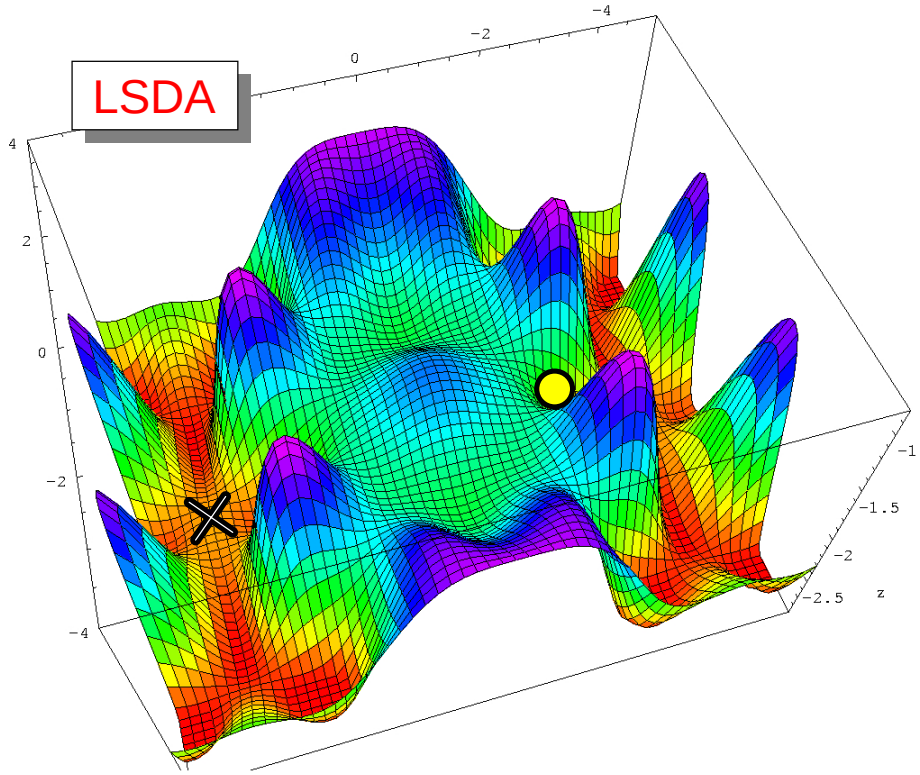
Ga-substitutional site

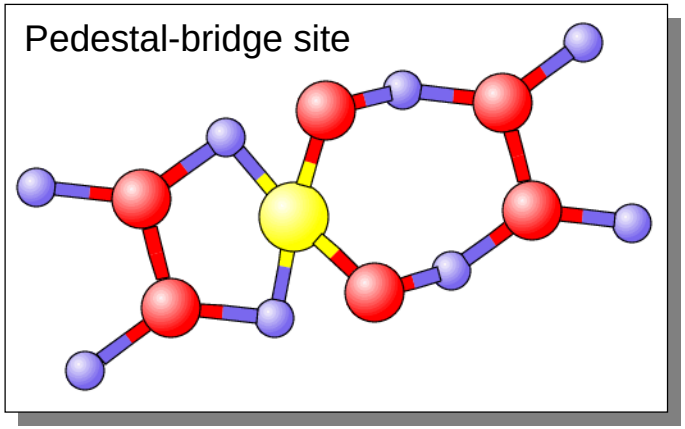


ΔE = -0.8 eV

Potential energy surfaces: LDA *vs.* LSDA

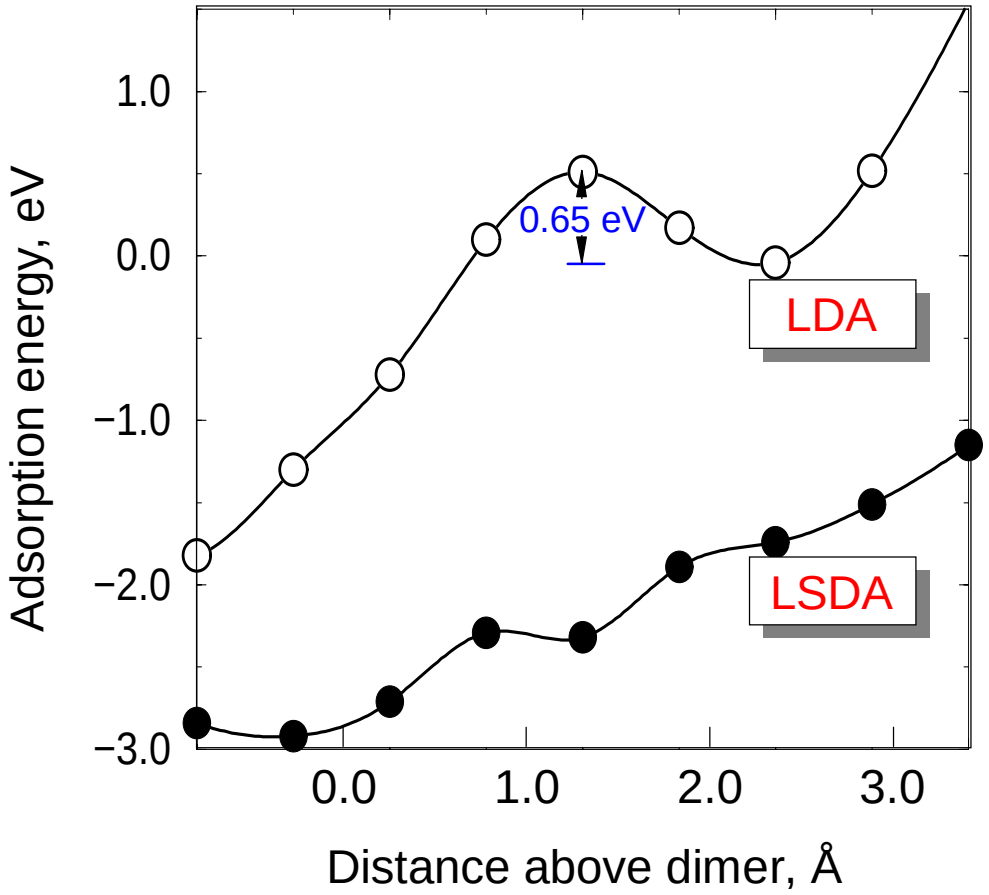


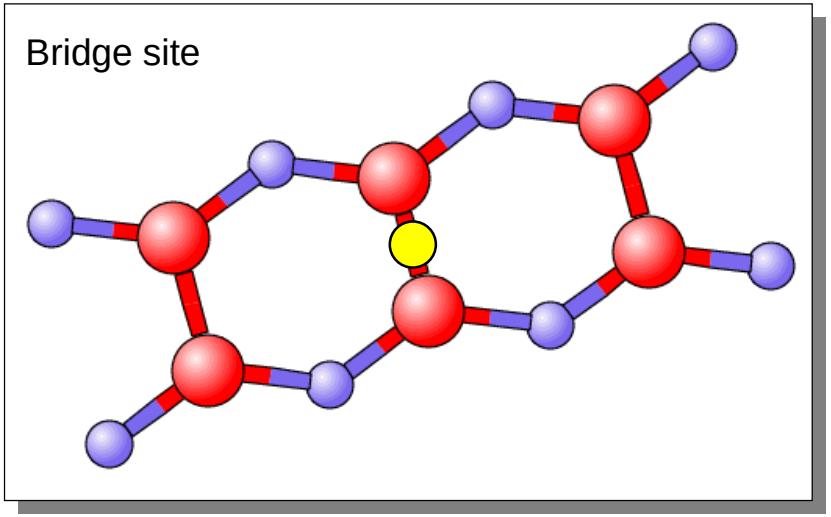




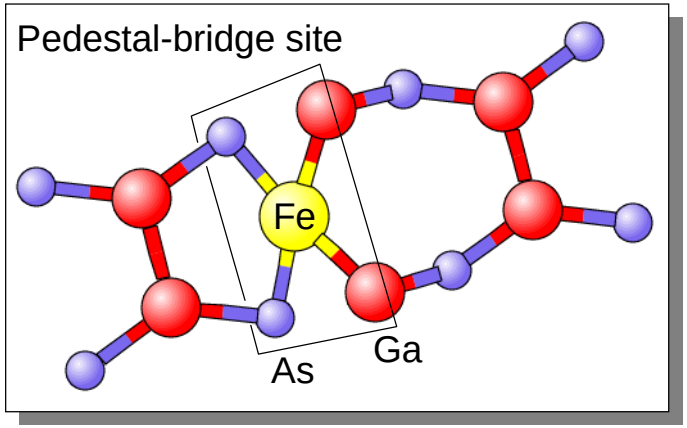
Dimer breaking and LDA *vs.* LSDA

Total energy of Fe above the bridge site





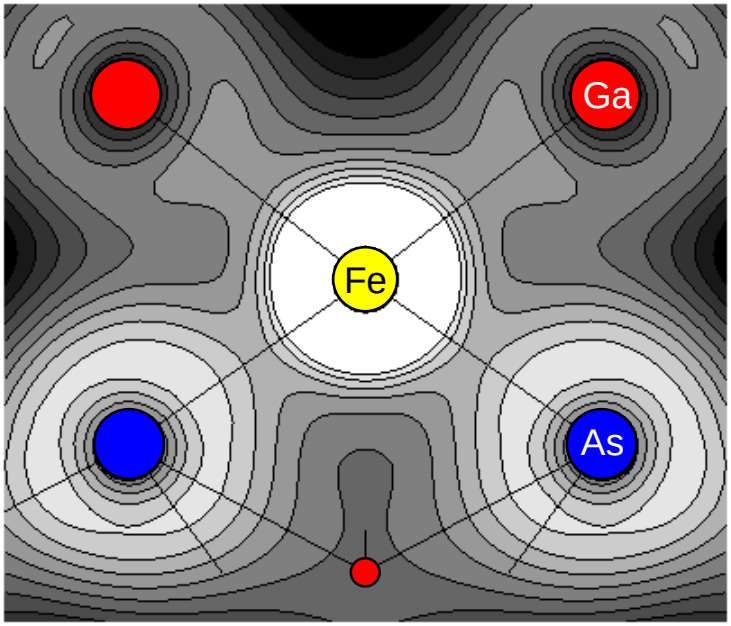
Does LSDA strengthen Fe-Ga/As bonds?

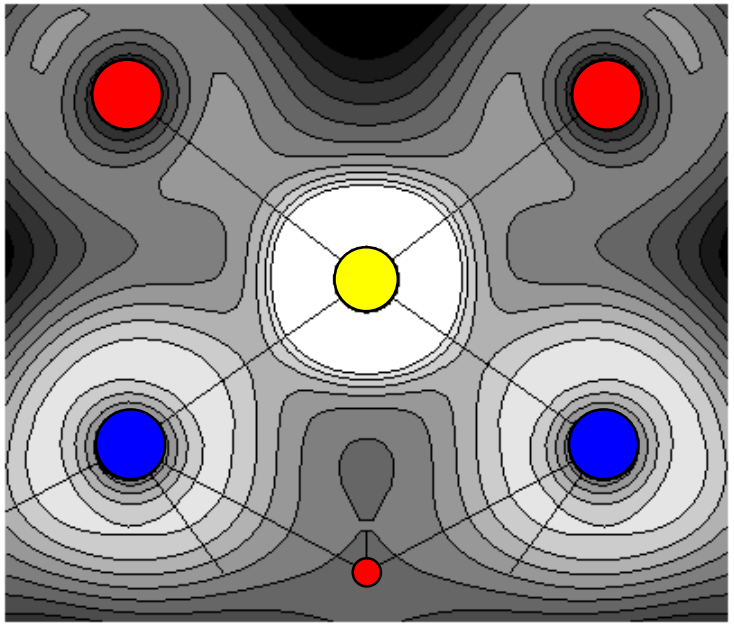


LDA

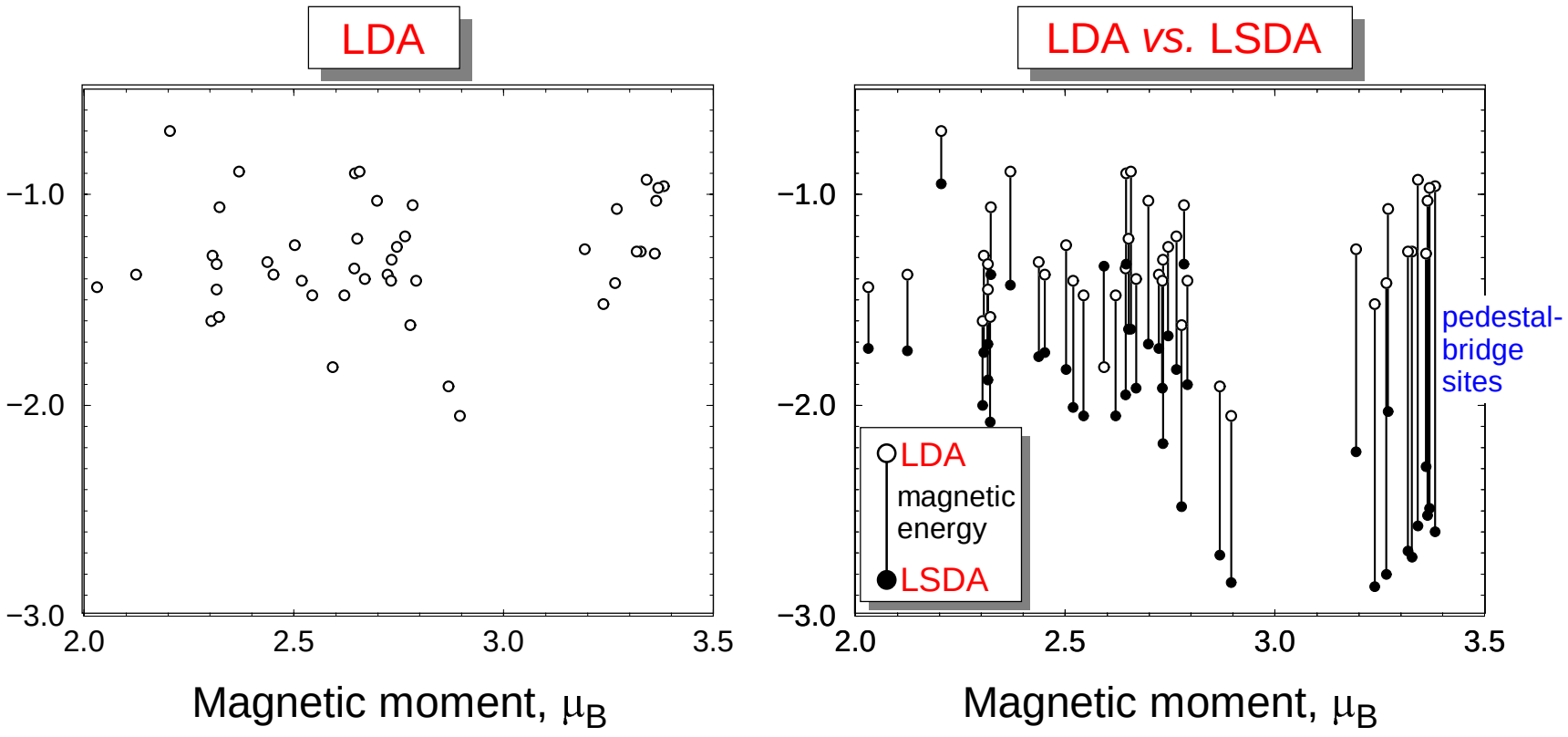
Valence electron density

LSDA





Adsorption energy *vs.* magnetic moment

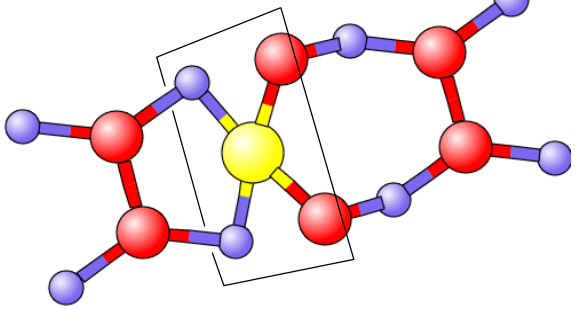


- Magnetic moments independent of non-magnetic (LDA) adsorption energy.
- Magnetic energy strongly dependent on magnetic moment.
- Largest magnetic energy gain for pedestal-bridge sites. Why?

Magnetic moment *vs.* adsorption site

Breaking bonds

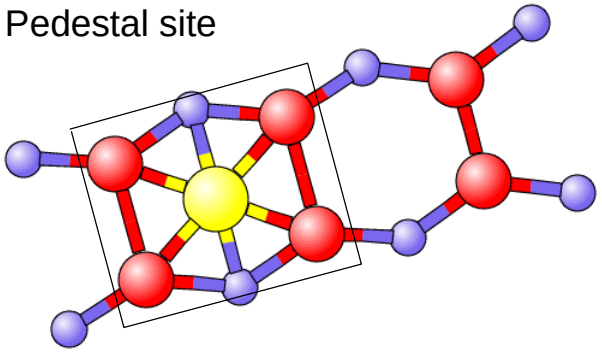
Pedestal-bridge site



ΔE_{mag} = -1.20 eV

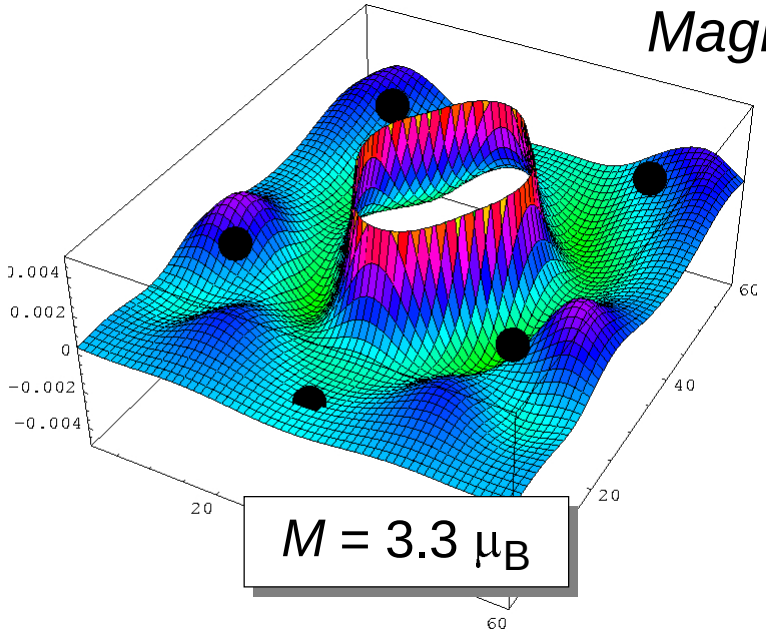
Intact bonds

Pedestal site

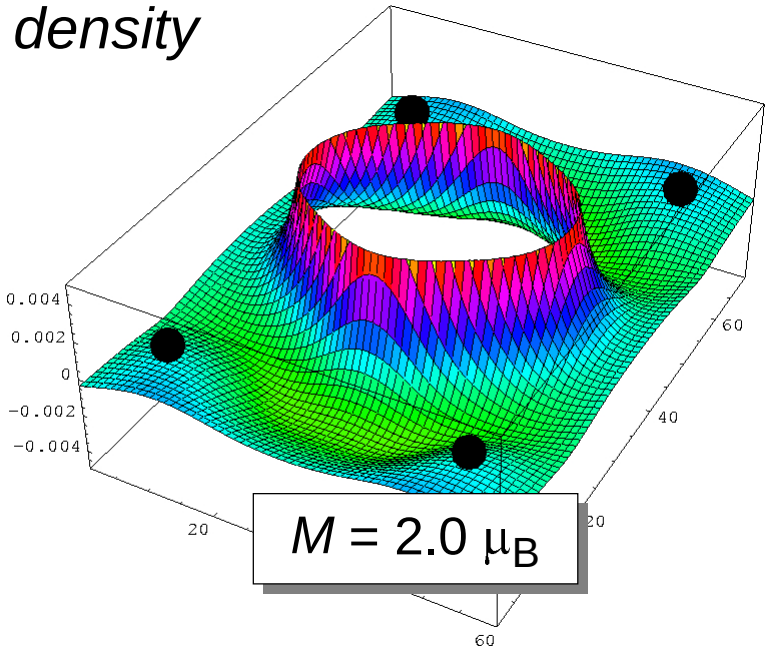


ΔE_{mag} = -0.03 eV

Magnetization density



M = 3.3 μ_B



M = 2.0 μ_B

Summary and outlook

Growth of Fe on Ga-rich GaAs(001)

- Fe adatoms easily "crack" Ga-Ga dimers to form stronger Fe-Ga dimers
- Fe-Ga dimers are strong traps, preventing Fe diffusion (esp. if Ga diffuses away)
- Next important phase: Formation of Fe-Fe dimers and release of first Ga monolayer
- Then what?

Generic features of Fe growth on GaAs

- Magnetic moments strongest when bonds are broken, weaker for intact bonds
- Magnetic effects strongly alter details of PES landscape

Next...

- Formation of first few Fe monolayers
- Role of temperature and flux rate on film structure
- Development of film magnetism as a function of structure, temperature, and flux